

netlognews

NETL's R&D newsletter

April 2013, Issue 29



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Cover image: NETL's new supercomputer in Morgantown, West Virginia, is one of the world's fastest and most energy efficient.

netlognews

newlognews is a quarterly newsletter highlighting recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.



CARNEGIE SCIENCE CENTER
One of the four Carnegie Museums of Pittsburgh

NETL Earns Carnegie Science Awards for Advanced Materials and Corporate Innovation

—For its leadership and innovation in science and technology, the National Energy Technology Laboratory has earned [two Carnegie Science Awards](#) from the Carnegie Science Center in Pittsburgh, PA. Representatives from NETL will receive the Advanced Materials Award and the Corporate Innovation Award at the 17th annual award ceremony to be held May 3, 2013, at the Carnegie Music Hall in Pittsburgh.

The Carnegie Science Center established the Carnegie Science Awards program in 1997 “to recognize and promote innovation in science and technology across western Pennsylvania.” The awards not only identify the innovators of today who make a global impact with their novel ideas and technologies, they also encourage tomorrow’s leaders in science, technology, engineering, and mathematics.

NETL’s platinum-chromium (Pt-Cr) alloy was selected for the Advanced Materials Award, which honors “accomplishments in materials science that create new materials or properties leading to significant business, economic, or societal benefits for the region.” Developed collaboratively by scientists from NETL and Boston Scientific, the Pt-Cr alloy solves many of the past problems surrounding traditional coronary stents.

A national resource centered in energy-rich Pittsburgh, [NETL-RUA](#) will receive the Corporate Innovation Award, given to “an organization or representative of an organization that develops and encourages an environment that promotes innovation in science or technology.” The Alliance combines the facilities, expertise, and resources of NETL with those of five world-renowned research universities: Carnegie Mellon, Penn State, the University of Pittsburgh, Virginia Tech, and West Virginia University. The Alliance is improving power generation efficiencies; reducing CO₂ separation costs; demonstrating CO₂ capture, utilization, and storage to reduce the environmental impact of fossil fuel use; and reducing the nation’s dependence on foreign energy supplies by investigating domestic alternatives, such as methane hydrates, deep drilling, shale gas, and enhanced oil recovery.



Gas pipeline employee.

NETL Participates in Community-Based Job Effort—[ShaleNET](#), a coalition of regional community colleges, has consulted NETL staff to gain a perspective on the science-based subject matter needed by workers in high-priority occupations in the natural gas drilling and production industry. In addition to basic science, the NETL panel recommended the workforce be schooled in geology, petroleum geology and engineering, environmental impacts and monitoring, process control, well logging, and materials engineering.

Working under a Community-Based Job Training Grant from the U.S. Department of Labor, ShaleNET has built and employed strong industry partnerships to define the structure of the industry, present and future labor needs, and training programs to meet those needs. Led by Westmoreland County Community College, ShaleNET is expanding existing certificate programs to provide training for upstream, midstream, and downstream operations jobs in shale gas fields in Pennsylvania, Ohio, West Virginia, and Texas. Coupled with a core curriculum, these certificates will lead to the accomplishment of Associate in Applied Science degrees from partner colleges. ShaleNET has invited NETL staff to participate with industry trainers in further refinement of the training curriculum designed to support the expanded certificate programs to be implemented during the 2013-2014 academic year.

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An image of an offshore oil rig.

Wellbore Cement Research Acclaimed at American Petroleum Institute Meeting—NETL scientist Dr. Barbara Kutchko presented selected results of her team's examination of offshore cementing practices to the American Petroleum Institute's (API) Subcommittee on Oil Well Cements (SC 10), which develops and maintains standards on various oil and gas wellbore cementing procedures for the U.S. petroleum industry. Building on NETL expertise and history in subsurface borehole cementing R&D, Dr. Kutchko's team initiated the work following the 2010 BP-Macondo spill in the Gulf of Mexico to improve understanding of the foamed cement systems commonly used there.

Delivered at the 2013 API Exploration & Production Winter Standards Meeting, the presentation introduced prominent members of the oil and gas industry to a recently published NETL Technical Report Series ([NETL-TRS-3-2012](#)) assessing the research needed to improve primary cement isolation of formations in deep offshore wells.

Wells in the Gulf of Mexico are being drilled in increasingly extreme environments, in water depths exceeding 9,000 feet and subsurface targets in excess of 20,000 feet below the seafloor. As a result, cement barriers in offshore wells are subject to a variety of temperature, pressure, and in situ fluid and formation conditions. Both the report and research were enthusiastically received and recognized as important work to help decrease the risk of loss of control or spill events in deep offshore systems.

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First Carbon Capture Simulation Initiative Toolset Licensed

The NETL led Carbon Capture Simulation Initiative (CCSI), a public-private partnership led by NETL, is developing, demonstrating, and deploying state-of-the-art computational tools to accelerate carbon capture technologies. CCSI meets an urgent need to take carbon capture concepts from the laboratory to the power plant more quickly at lower cost and with reduced risk. The CCSI Toolset works with commercial and open-source software currently in use by industry and includes new software tools developed to fill technology gaps. The tools are highly versatile. In addition to their use in developing carbon capture technologies, they can be used to accelerate the development of technologies for the chemical and petrochemical industries.

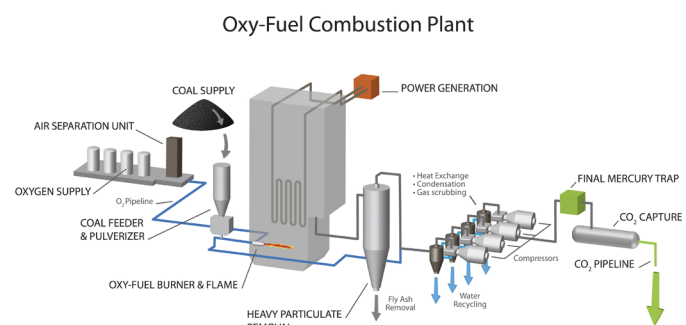
CCSI recently finalized its initial licensing agreements allowing GE, Alstom Power, and Phillips 66 to apply the CCSI Toolset in developing their own carbon capture and related processes. These initial licenses are the result of intense industry interest in gaining early access to the CCSI Toolset that prompted the technical team to move forward its initial release by over a year.

The [first release consists of new tools](#) for process synthesis and optimization to help identify promising concepts more quickly, new physics-based models of potential capture equipment and processes that will reduce the time to design and troubleshoot new systems, a framework to quantify the uncertainty of model predictions, and various enabling tools that will provide new capabilities such as creating reduced models (RMs) from reacting multiphase flow simulations and running thousands of process simulations concurrently for optimization and uncertainty quantification.

CCSI recently began its third year of development and will be focusing on creating physics-based models for new types of carbon capture systems as well as continuing to develop computational tools broadly applicable to the full breadth of potential capture technologies.

The CCSI technical team includes researchers at NETL, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Pacific Northwest National Laboratory, Boston University, Carnegie Mellon University, Princeton University, West Virginia University, the University of Texas, and the University of Utah.

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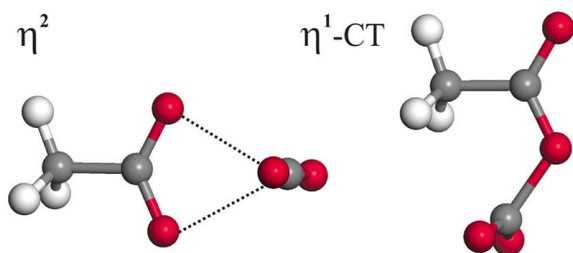


Research for Selective Oxidation in Oxy-fuel Combustion Environments

Essentially all alloys and coatings that resist corrosion at high temperature are able to form a protective (slowly-growing and adherent) oxide layer by a process known as selective oxidation. NETL researchers have collaborated in developing oxy-fuel combustion systems where fossil fuels are burned in a mixture of recirculated flue gas and oxygen rather than in air. This research has caused renewed interest in the effects of water vapor and steam on alloy oxidation.

Working jointly with researchers at the University of Pittsburgh, NETL-Regional University Alliance partner, NETL scientists measured and tracked hydrogen that evolves from the oxidation of iron in steam. Hydrogen is thought to increase internal oxidation within alloys, and measuring the fraction injected into the alloy is needed to validate such mechanisms. In addition, the collaborators examined interactions between vapor and carbon dioxide, which can either allow or prevent alloy carburization from occurring. Results of this research will appear in an issue of the Springer publication, *Oxidation of Metals* ([doi:10.1007/s11085-012-9349-8](https://doi.org/10.1007/s11085-012-9349-8)).

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The η^2 and η^1 -CT structures of the acetate- CO_2 complex.

Publication Addresses the Optimization of Ionic Liquids for Carbon Capture

Ionic liquids (ILs), which can be thought of as salts that are molten at room temperature, are being studied for use as part of CO_2 adsorption and/or separation technologies. These applications depend on having strong interactions between the CO_2 and the ions of the IL. In order for significant advances to occur in this area of research, the interaction between the CO_2 and each IL must be understood and described with accuracy.

Despite significant experimental efforts, many of the underlying factors that govern the interaction of CO_2 with an ionic liquid remain unknown. Such limitations, however, can be addressed using computational methods that apply first-principles molecular orbital calculations to obtain an accurate description of these interactions at the molecular level. An NETL-authored [paper](#) published by the American Chemical Society in *The Journal of Physical Chemistry A* (Vol. 16 (2012), No. 47, pp. 11643-11650) elucidates the complex nature of the interactions between CO_2 and acetate ions, a prototype anion present in many of the ionic liquids under evaluation for CO_2 separation technologies.

The importance of this study resides in providing a clear understanding of the complex nature of CO_2 -acetate ion [interaction](#). Also important is establishing the energetic and structural benchmark data that can be used for further development of new ionic liquids compositions, and development of larger-scale simulation methods for bulk ionic liquids. An important result highlighted in this paper is that many popular density functional theory (DFT) methods do not accurately describe the acetate- CO_2 interaction.

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NETL's High-Performance Computer for Energy and the Environment (HPCEE) located in Morgantown, WV.

NETL's New Supercomputer Ranked Among the World's Top 100

One of the world's fastest, most energy-efficient supercomputers is up and running at NETL's facility in Morgantown, WV. The High-Performance Computer for Energy and the Environment ([HPCEE](#)) is not only on the TOP 500 list as one of the top 100 supercomputers in the world—currently ranked at 55—but it is also one of the most energy efficient for its size.

Housed at NETL's Simulation-Based Engineering User Center, the supercomputer is a 503 TFlops (trillion floating-point operations per second) computer that enables the simulation of phenomena that are difficult or impossible to measure, such as coal jet penetration into a gasifier. With capabilities for running modeling tools at various scales ranging from molecules, to devices, to entire power plants and natural fuel reservoirs, the HPCEE is the backbone for providing enhanced visualization, data analysis, and data storage capabilities.

All of the computational, visualization, network hardware, and primary storage servers are installed in a Silicon Graphics ICE Cube® Air modular data center. This datacenter provides the HPCEE one of the lowest power utilization efficiency (PUE) infrastructures available, with a range of 1.01 to 1.1 PUEs. To date, the HPCEE has one of the lowest recorded PUEs achieved in the industry, using only one percent of total electrical consumption to cool the equipment—far surpassing the DOE Office of the Chief Information Officer's standard of 40 percent. The increase in efficiency translates to electrical energy cost savings of approximately \$450,000 annually.



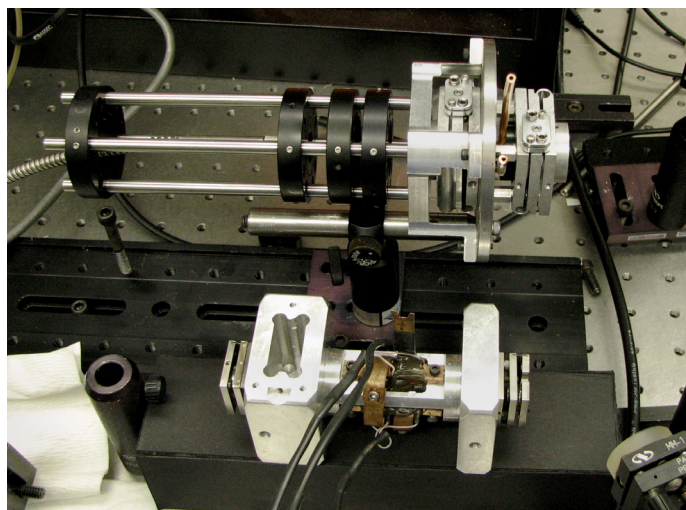
NETL's membrane screening system accelerates membrane testing by a factor of 12.

NETL Files Patent Application for High-Speed Membrane Screening Device

—Membranes offer a potential low-maintenance and economical method for gas separations from power plant flue gas streams. Polymer membranes and supported liquid membranes show great promise to solve problems in the area of clean energy production. Carbon dioxide, a greenhouse gas, is a principal by-product of energy production from fossil fuels. Capturing CO₂ from power plant flue gas streams is critical to the goal of reducing the nation's carbon footprint and preserving the environment. Currently, no technology can meet the goals for carbon capture as set forth by the U.S. Department of Energy. These goals are 90 percent capture of the CO₂ with a less than 35 percent increase in the cost of energy.

The optimization of membranes for any application requires researchers to characterize the performance of large numbers of sample materials, but traditional approaches can take days or weeks to determine the transport properties of a single sample. NETL researchers have now demonstrated and filed a patent for a [unique device](#) capable of parallel-testing up to 16 samples for permeability and mixed gas selectivity, quadrupling the Laboratory's capacity for screening candidate membrane materials for carbon capture and oxygen purification.

Contacts: [Dave Luebke](#), 412-386-4118



The image shows two versions of passively Q-switched lasers. The larger laser nearer the top of the photo is an end-pumped excitation laser, and the laser nearer the bottom is a side-pumped version used for LIBS analysis. At the top of the photo is the power supply.

Scientists Improve Method for Laser-Induced Breakdown Spectroscopy (LIBS)

—The nanosecond laser output pulse used in LIBS systems is normally produced with active Q-switched lasers, which are expensive and can require precisely timed high voltage signals. With passive Q-switching, control signals for operating and producing LIBS output would be eliminated and/or greatly simplified, reducing system cost and complexity. NETL scientists devised the use of a passive feedback sensor to pick up the spike of intracavity photon flux scattering out of the laser with each pulse. The sensor actuates a set of delay functions in a controller that triggers a spectrometer at the precise instant when the light returning from the laser target is characteristic of the elements atomized there.

This invention will allow for precise control with fewer control lines and less expensive parts. The laser can be miniaturized into a monolithic optical unit while still providing sufficient output to produce laser sparks. The laser can be pumped with a bank of diode lasers or a vertical-cavity surface-emitting laser (VCSEL) to maintain good mode and output beam quality. The use of the passively q-switched laser will reduce system cost by thousands of dollars.

This invention can also be used to report the output pulse energy of the laser system to the LIBS analysis system.

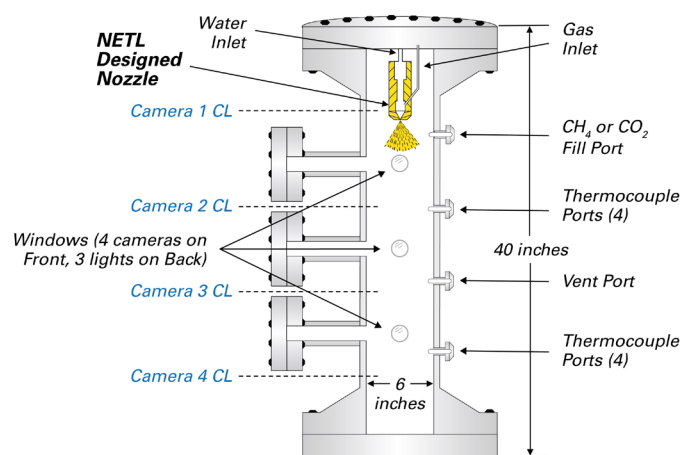
Maintaining consistent output pulse energy levels and/or at least accurately reporting the variations can help reduce errors within the LIBS analysis process. The measurement of Q-switch delay can also be used to calibrate and report output pulse energy.

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Methane hydrate can store 164 times its volume in gas (at standard temperature and pressure) and survives at atmospheric pressure and temperatures (-10 to -20 °C) routinely used for the commercial transport of frozen food. A process for rapid and continuous formation of methane hydrate could offer a safer, more cost-effective method for storing and transporting methane compared with conventional compressed and liquefied natural gas.

This technology may be applicable to carbon dioxide sequestration, separation of mixed gases (e.g., natural gas streams containing carbon dioxide and other gases impacting high methane content), cold energy storage, transportation fuels, and desalination processes.

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NETL-designed Rapid Hydrate Formation Nozzle in the 15-liter Cell.

Rapid Hydrate Formation Apparatus Nozzle Patent Issued

—Methane hydrate—molecules of natural gas trapped in an ice-like cage of water molecules—represents a potentially vast methane resource for both the United States and the world. Recent discoveries of methane hydrate in arctic and deep-water marine environments have highlighted the need for a better understanding of this substance as a natural storehouse of carbon and as a potential energy resource.

Methane hydrate formation typically takes anywhere from 6 hours to several days or weeks under laboratory conditions. NETL scientists have invented a nozzle design that allows the instantaneous and continuous formation of gas hydrates from a two-phase mixture of water and hydrate-forming gas. Patent No. 8,354,565 was recently issued for this technology. As applied to methane, the invention could radically transform the economics of shale gas and landfill gas development, transportation, and purification.

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3.	Van Essendelft, D. T.; Zhou, X.; Kang, B. S. March 2013. Grindability Determination of Torrefied Biomass Materials Using the Hybrid Work Index, <i>Fuel</i> , 105, 103-11.
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9.	Tafen, D. N.; Miller, J.B.; Dogan, O.N., et al. February 2013. Oxygen-Induced Y Surface Segregation in a CuPdY Ternary Alloy, <i>Surface Science</i> , 608, 61-66.
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13.	Kauffman, Douglas R.; Alfonso, Dominic; Matranga, Christopher, et al. January 3, 2013. Photomediated Oxidation of Atomically Precise Au-25(SC ₂ H ₄ Ph)(18)(-) Nanoclusters, <i>J. Phys. Chem. Ltrs.</i> , 4 (1) 195-202.

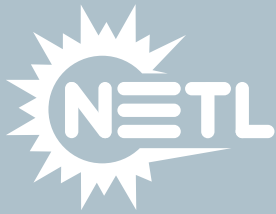
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25.	Arroyave, Raymundo; Gao, Michael. December 2012. Gas-Alloy Interactions at Elevated Temperatures, 64 (12) 1425-1425.

Patents Issued This Quarter

1.	Rapid Gas Hydrate Formation Process. Thomas Brown, Charles E. Taylor, Alfred J. Unione, 8354565 , issued January 1, 2013.
2.	Fabrication of Fiber Supported Ionic Liquids and Methods of Use. David Luebke and Shan Wickramanayake, 8383026 , issued February 26, 2013.
3.	Method of Particle Trajectory Recognition in Particle Flows of High Particle Concentration Using a Candidate Trajectory Tree Process with Variable Search Areas. Franklin D. Schaffer, 8391552 , issued March 5, 2013.

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